

An asymptotic expansion for the Stieltjes constants

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Abstract

The Stieltjes constants γ_n appear in the coefficients in the Laurent expansion of the Riemann zeta function $\zeta(s)$ about the simple pole $s = 1$. We present an asymptotic expansion for γ_n as $n \rightarrow \infty$ based on the approach described by Knessl and Coffey [Math. Comput. **80** (2011) 379–386]. A truncated form of this expansion with explicit coefficients is also given. Numerical results are presented that illustrate the accuracy achievable with our expansion.

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1. Introduction

The Stieltjes constants γ_n appear in the coefficients in the Laurent expansion of the Riemann zeta function $\zeta(s)$ about the point $s = 1$ given by

$$\zeta(s) = \frac{1}{s-1} + \sum_{n=0}^{\infty} \frac{(-)^n}{n!} \gamma_n (s-1)^n,$$

where $\gamma_0 = 0.577216\dots$ is the well-known Euler-Mascheroni constant. Some historical notes and numerical values of γ_n for $n \leq 20$ are given in [3]. Recent high-precision evaluations of γ_n based on numerical integration have been described in [5, 8]. In [5], Keiper lists various γ_n up to $n = 150$, whereas in [8], Kreminski has computed values to several thousand digits for $n \leq 10^4$ and for further selected values (accurate to 10^3 digits) up to $n = 5 \times 10^4$. All values up to $n = 10^5$ have been computed by Johansson in [4] to about 10^4 digits.

Upper bounds for $|\gamma_n|$ in the form

$$|\gamma_n| \leq \{3 + (-)^n\} \frac{\lambda_n \Gamma(n)}{\pi^n},$$

have been obtained by Berndt [1] with $\lambda_n = 1$, and by Zhang and Williams [13] with $\lambda_n = (2/n)^n \pi^{-\frac{1}{2}} \Gamma(n + \frac{1}{2}) \sim \sqrt{2}(2/e)^n$ for $n \rightarrow \infty$. On the other hand, Matsuoka [9] has shown that

$$|\gamma_n| \leq 10^{-4} e^{n \log \log n} \quad (n \geq 10).$$

However, all these bounds grossly overestimate the growth of $|\gamma_n|$ for large values of n . An asymptotic approximation for γ_n has recently been given by Knessl and Coffey [6] in the form

$$\gamma_n \sim \frac{Be^{nA}}{\sqrt{n}} \cos(na + b) \quad (n \rightarrow +\infty), \quad (1.1)$$

where A , B , a and b are functions that depend weakly on n ; see Section 2 for the definition of these quantities. Knessl and Coffey have verified numerically that for $n \leq 3.5 \times 10^4$ the above formula accounts for the asymptotic growth and oscillatory pattern of γ_n , with the exception of $n = 137$ where the cosine factor in (1.1) becomes very small.

The aim in this note is to extend the analysis in [6] to generate an asymptotic expansion for γ_n as $n \rightarrow +\infty$. The coefficients in this expansion are determined numerically by application of Wojdyło's formulation [14] for the coefficients in the expansion of a Laplace-type integral. An explicit evaluation of the coefficients is obtained in the case of the expansion truncated after three terms. This approximation is extended to the more general Stieltjes constants $\gamma_n(\alpha)$ appearing in the Laurent expansion of the Hurwitz zeta function $\zeta(s, \alpha)$. Numerical results are presented in Section 3 to demonstrate the accuracy of our expansion compared to that in (1.1).

2. Asymptotic expansion for γ_n

We start with the integral representation for $n \geq 1$ given in [13]

$$\gamma_n = \int_1^\infty B_1(x - [x]) \frac{\log^{n-1} x}{x^2} (n - \log x) dx,$$

where $B_1(x - [x]) = -\sum_{j=1}^\infty \frac{\sin 2\pi jx}{\pi j}$ is the first periodic Bernoulli polynomial. With the change of variable $t = \log x$, we obtain [6, Eq. (2.3)]

$$\gamma_n = -\Im \left\{ \sum_{k=1}^\infty \frac{1}{\pi k} \int_0^\infty \exp[2\pi i k e^t + n \log t - t] \left(\frac{n}{t} - 1 \right) dt \right\}.$$

Following the approach used in [6], we define

$$\psi_k(t) \equiv \psi_k(t; n) = -\frac{2\pi i k}{n} e^t - \log t, \quad f(t) \equiv f(t; n) = \frac{e^{-t}}{t} \left(1 - \frac{t}{n} \right) \quad (2.1)$$

and write

$$\gamma_n = -\Im \sum_{k=1}^\infty J_k, \quad J_k := \frac{n}{\pi k} \int_0^\infty e^{-n\psi_k(t)} f(t) dt. \quad (2.2)$$

We employ the method of steepest descents to estimate the integrals J_k for large values of n . Saddle points of the exponential factor occur at the zeros of $\psi'_k(t) = 0$; that is, they satisfy

$$te^t = \frac{ni}{2\pi k}. \quad (2.3)$$

There is an infinite string of saddle points, which is approximately parallel to the imaginary t -axis, given by [6]

$$t_m = \log \frac{n}{2\pi k} - \log \log n + (2m + \tfrac{1}{2})\pi i + O\left(\frac{\log \log n}{\log n}\right)$$

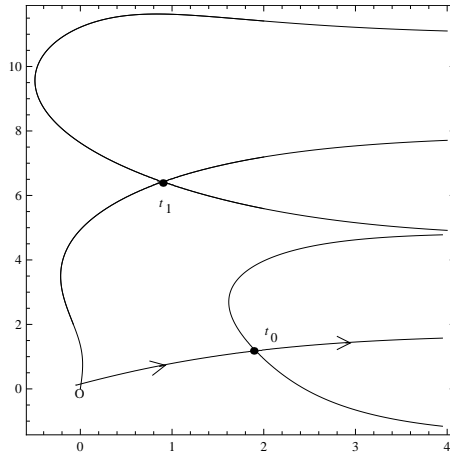


Figure 1: Paths of steepest descent and ascent through the saddles t_0 and t_1 when $n = 100$ and $k = 1$. The steepest paths through the saddle t_{-1} (not shown) in the lower half-plane are similar to those through t_1 . The arrows indicate the direction of integration.

for $m = 0, \pm 1, \pm 2, \dots$ and large n . For fixed k and m , the value of $\Re \psi_k(t_m)$ is then

$$-\Re \psi_k(t_m) = \log \log n - \frac{1}{\log n} (1 + \log (2\pi k \log n)) + O((\log n)^{-2})$$

as $n \rightarrow \infty$, where the dependence on m is contained in the order term. This shows that the heights of the saddles corresponding to $k \geq 2$ are exponentially smaller as $n \rightarrow \infty$ than the saddle with $k = 1$, so that to within exponentially small correction terms we may neglect the contribution in (2.2) arising from k values corresponding to $k \geq 2$; but see the discussion in Section 3. From hereon, we shall drop the subscript k and write $\psi_1(t) \equiv \psi(t)$.

Typical paths of steepest descent and ascent through the saddles t_0 and t_1 are shown in Fig. 1. Steepest descent and ascent paths terminate at infinity in the right-half plane in the directions $\Im(t) = (2j + \frac{1}{2})\pi$ and $\Im(t) = (2j + \frac{3}{2})\pi$ ($j = 0, \pm 1, \pm 2, \dots$), respectively. The steepest descent paths through t_0 and t_1 emanate from the origin and pass to infinity in the directions $\Im(t) = \frac{1}{2}\pi$ and $\frac{5}{2}\pi$, respectively. Similarly, the steepest descent path through t_{-1} (not shown) emanates from the origin and passes to infinity in the direction $\Im(t) = -\frac{3}{2}\pi$. The integration path in (2.2) can then be deformed to pass through the saddle t_0 as shown in Fig. 1.

Application of the method of steepest descents (see, for example, [10, p. 127] and [11, p. 14]) then yields

$$J_1 \sim \frac{n}{\pi} \frac{\sqrt{2\pi} e^{-n\psi(t_0)-t_0}}{t_0(-\psi''(t_0))^{1/2}} \left(1 - \frac{t_0}{n}\right) \sum_{s=0}^{\infty} \frac{\hat{c}_{2s}(\frac{1}{2})_s}{n^{s+1/2}}, \quad (2.4)$$

where $(a)_s = \Gamma(a+s)/\Gamma(a)$ is the Pochhammer symbol and $\hat{c}_0 = 1$. The normalised coefficients \hat{c}_{2s} can be obtained by an inversion process and are listed for $s \leq 4$ in [2, p. 119] and for $s \leq 2$ in [11, p. 13]; see below. Alternatively, they can be obtained by an

expansion process to yield Wojdylo's formula [14] given by

$$\hat{c}_s = \alpha_0^{-s/2} \sum_{k=0}^s \frac{\beta_{s-k}}{\beta_0} \sum_{j=0}^k \frac{(-)^j (\frac{1}{2}s + \frac{1}{2})_j}{j! \alpha_0^j} \mathcal{B}_{kj}; \quad (2.5)$$

see also [12, p. 25]. Here $\mathcal{B}_{kj} \equiv \mathcal{B}_{kj}(\alpha_1, \alpha_2, \dots, \alpha_{k-j+1})$ are the partial ordinary Bell polynomials generated by the recursion¹

$$\mathcal{B}_{kj} = \sum_{r=1}^{k-j+1} \alpha_r \mathcal{B}_{k-r, j-1}, \quad \mathcal{B}_{k0} = \delta_{k0},$$

where δ_{mn} is the Kronecker symbol, and the coefficients α_r and β_r appear in the expansions

$$\psi(t) - \psi(t_0) = \sum_{r=0}^{\infty} \alpha_r (t - t_0)^{r+2}, \quad f(t) = \sum_{r=0}^{\infty} \beta_r (t - t_0)^r \quad (2.6)$$

valid in a neighbourhood of the saddle $t = t_0$.

Following [6], we put $t_0 = u + iv$, where u, v are real, and write $-\psi(t_0) = A + ia$, where

$$\left. \begin{aligned} A : &= \Re(\log t_0 - 1/t_0) = \frac{1}{2} \log(u^2 + v^2) - \frac{u}{u^2 + v^2}, \\ a : &= \Im(\log t_0 - 1/t_0) = \arctan\left(\frac{v}{u}\right) + \frac{v}{u^2 + v^2}. \end{aligned} \right\} \quad (2.7)$$

We have $\psi''(t_0) = (1 + t_0)/t_0^2$ and accordingly define²

$$B := 2\sqrt{2\pi} \left| \frac{t_0}{\sqrt{1+t_0}} \right|, \quad b := \frac{1}{2}\pi - v - \arctan\left(\frac{v}{1+u}\right). \quad (2.8)$$

A simple calculation using (2.3) with $k = 1$ shows that

$$\tan v = \frac{u}{v}, \quad e^{-u} = \frac{2\pi|t_0|}{n}. \quad (2.9)$$

Then, from (2.2) with $k = 1$, (2.4) and the second relation in (2.9), we find upon incorporating the factor $1 - t_0/n$ into the asymptotic series that

$$\gamma_n \sim \frac{B e^{nA}}{\sqrt{n}} \Re \left\{ e^{i(na+b)} \sum_{s=0}^{\infty} \frac{c'_{2s}(\frac{1}{2})_s}{n^s} \right\},$$

where

$$c'_{2s} = \hat{c}_{2s} - \frac{2t_0}{2s-1} \hat{c}_{2s-2} \quad (s \geq 1). \quad (2.10)$$

If we now introduce the real and imaginary parts of the coefficients \hat{c}_{2s} by

$$c'_{2s} := C_s + iD_s \quad (s \geq 1), \quad C_0 = 1, \quad D_0 = 0, \quad (2.11)$$

where we recall that C_s and D_s contain an n -dependence, then we have the expansion of γ_n given by the following theorem.

¹For example, this generates the values $\mathcal{B}_{41} = \alpha_4$, $\mathcal{B}_{42} = \alpha_3^2 + 2\alpha_1\alpha_3$, $\mathcal{B}_{43} = 3\alpha_1^2\alpha_2$ and $\mathcal{B}_{44} = \alpha_1^4$.

²In [6], the quantity $\frac{1}{2}\pi - v$ appearing in the definition of b is written as $\arctan(v/u)$ by virtue of the first relation in (2.9).

Theorem 1. *Let the quantities A , B , a and b , and the coefficients C_s , D_s , be as defined in (2.7), (2.8) and (2.11). Then, neglecting exponentially smaller terms, we have*

$$\gamma_n \sim \frac{Be^{nA}}{\sqrt{n}} \left\{ \cos(na + b) \sum_{s=0}^{\infty} \frac{C_s(\frac{1}{2})_s}{n^s} - \sin(na + b) \sum_{s=1}^{\infty} \frac{D_s(\frac{1}{2})_s}{n^s} \right\} \quad (2.12)$$

as $n \rightarrow \infty$.

We note that to leading order $A \sim \log \log n$ and $B \sim (8\pi \log n)^{1/2}$ for large n .

A simpler form of the expansion (2.12) can be given by truncating the above series at $s = 2$ and use of the form of the normalised coefficients \hat{c}_{2s} in (2.4) expressed in the form

$$\begin{aligned} \hat{c}_2 &= \frac{1}{2\psi''(t_0)} \{2F_2 - 2\Psi_3 F_1 + \frac{5}{6}\Psi_3^2 - \frac{1}{2}\Psi_4\}, \\ \hat{c}_4 &= \frac{1}{(2\psi''(t_0))^2} \left\{ \frac{2}{3}F_4 - \frac{20}{9}\Psi_3 F_3 + \frac{5}{3}(\frac{7}{3}\Psi_3^2 - \Psi_4)F_2 - \frac{35}{9}(\Psi_3^3 - \Psi_3\Psi_4 + \frac{6}{35}\Psi_5)F_1 \right. \\ &\quad \left. + \frac{35}{9}(\frac{11}{24}\Psi_3^4 - \frac{3}{4}(\Psi_3^2 - \frac{1}{6}\Psi_4)\Psi_4 + \frac{1}{5}\Psi_3\Psi_5 - \frac{1}{35}\Psi_6) \right\} \end{aligned}$$

where, for brevity, we have defined

$$\Psi_m := \frac{\psi^{(m)}(t_0)}{\psi''(t_0)} \quad (m \geq 3), \quad F_m := \frac{f^{(m)}(t_0)}{f(t_0)} \quad (m \geq 1);$$

see [2, p. 119], [11, pp. 13–14].

From (2.1) and (2.10), use of *Mathematica* shows that

$$c'_2 = \frac{\wp_2(t_0)}{12(1+t_0)^3} + \frac{(4+3t_0)t_0^2}{n(1+t_0)^2} + O(n^{-2}), \quad c'_4 = \frac{\wp_4(t_0)}{864(1+t_0)^6} + O(n^{-1}),$$

where

$$\begin{aligned} \wp_2(t_0) &= 2 - 18t_0 - 20t_0^2 - 3t_0^3 + 2t_0^4, \\ \wp_4(t_0) &= 4 - 72t_0 - 332t_0^2 - 8028t_0^3 - 19644t_0^4 - 20280t_0^5 - 9911t_0^6 - 1884t_0^7 + 4t_0^8. \end{aligned}$$

Then we obtain the following result.

Theorem 2. *Let the quantities A , B , a and b be as defined in (2.7) and (2.8). Then, with*

$$c_1 + id_1 = \frac{\wp_2(t_0)}{24(1+t_0)^3}, \quad c_2 + id_2 = \frac{\wp_4(t_0)}{1152(1+t_0)^6} + \frac{(4+3t_0)t_0^2}{2(1+t_0)^2},$$

where c_s , d_s ($s = 1, 2$) are real (and independent of n) and t_0 is the saddle point given by the principal solution of (2.3) with $k = 1$, we have the asymptotic approximation

$$\gamma_n \sim \frac{Be^{nA}}{\sqrt{n}} \left\{ \cos(na + b) \left(1 + \frac{c_1}{n} + \frac{c_2}{n^2} \right) - \sin(na + b) \left(\frac{d_1}{n} + \frac{d_2}{n^2} \right) \right\} \quad (2.13)$$

as $n \rightarrow \infty$.

We remark that the expansion of the integrals J_k for fixed $k \geq 2$ follows the same procedure. If we still refer to the real and imaginary parts of the contributory saddle t_0 (when $k \geq 2$) as u and v , the second relation in (2.9) is now replaced by $e^{-u} = 2\pi k|t_0|/n$. It then follows that the form of the expansion for $-\Im J_k$ is given by (2.12), provided the quantities A , B , a and b , and the coefficients C_s , D_s , are interpreted as corresponding to the saddle t_0 with the k -value under consideration.

3. Numerical results and concluding remarks

We discuss numerical computations carried out using the expansions given in Theorems 1 and 2. For a given value of n the saddle t_0 is computed from (2.3) with $k = 1$ to the desired accuracy. *Mathematica* is used to determine the coefficients α_r and β_r in (2.6) for $0 \leq r \leq 2s_0$, where in the present computations $s_0 = 6$. The coefficients C_s and D_s can then be calculated for $0 \leq s \leq s_0$ from (2.5), (2.10) and (2.11).

We display the computed values of C_s and D_s for two values of n in Table 1. We repeat that these coefficients contain an n -dependence and so have to be computed for each value of n chosen. In Table 2, the values of the absolute relative error in the computation of γ_n from the expansion (2.12) are presented as a function of the truncation index s for several values of n .

Table 1: Values of the coefficients C_s and D_s (to 10 dp) for $1 \leq s \leq 6$ for two values of n .

s	$n = 100$		$n = 1000$	
	C_s	D_s	C_s	D_s
1	-0.3158578918	+0.1626819326	-0.0885061806	+0.1958085240
2	-2.9096870797	-2.1947177121	-6.5840165991	-2.6459812815
3	-0.3804847598	-3.3953890569	-9.4682639154	-10.09635962642
4	+1.4820479884	-0.1130053628	-1.3074432243	-11.31040992292
5	-0.2630549338	+0.9253656779	+4.9469591967	-1.67819725309
6	-0.3783700609	-0.3119889058	+0.8180579543	+3.98701271605

The case $n = 137$ has been included in Table 2 since this corresponds to the factor $\cos(na + b)$ possessing the very small value $\simeq 1.69881 \times 10^{-4}$. The leading term approximation in (1.1), and (2.12) (with $s = 0$), yields an incorrect sign, namely $+3.89874 \times 10^{27}$ when $\gamma_{137} = -7.99522199 \dots \times 10^{27}$. According to [4], this is the only instance for $n \leq 10^5$ when the leading approximation produces the wrong sign. It is seen that inclusion of the higher order correction terms with $s \leq 6$ yields a relative error of order 10^{-10} in this case. When $n = 10^5$, [4] gives the value

$$\gamma_{100000} = 1.99192730631254109565822724315 \dots \times 10^{83432}.$$

The expansion (2.12) for this value of n with truncation index $s = 6$ is found to yield a relative error of order 10^{-30} ; that is, the expansion correctly reproduces all the digits displayed above.

Table 2: Values of the absolute relative error in the computation of γ_n from (2.12) as a function of the truncation index s for different n .

s	$n = 75$	$n = 100$	$n = 137$	$n = 1000$
0	1.759×10^{-3}	1.412×10^{-3}	—	1.597×10^{-4}
1	6.503×10^{-4}	3.226×10^{-4}	2.701×10^{-1}	2.649×10^{-6}
2	1.244×10^{-5}	4.472×10^{-6}	8.775×10^{-2}	4.125×10^{-9}
3	3.063×10^{-7}	9.370×10^{-8}	3.811×10^{-5}	7.711×10^{-11}
4	2.535×10^{-9}	7.850×10^{-10}	2.183×10^{-6}	2.026×10^{-13}
5	5.101×10^{-10}	9.022×10^{-11}	1.248×10^{-8}	6.157×10^{-16}
6	1.850×10^{-11}	1.982×10^{-12}	9.415×10^{-10}	2.743×10^{-18}

Table 3: Values of the absolute relative error in the computation of γ_n from (2.12) with $k = 1$ and $k \leq 2$ as a function of the truncation index s for $n = 25$.

s	$k = 1$	$k \leq 2$
0	1.051×10^{-2}	1.052×10^{-2}
1	2.909×10^{-3}	2.894×10^{-3}
2	2.608×10^{-4}	2.460×10^{-4}
3	2.390×10^{-6}	1.723×10^{-5}
4	1.518×10^{-5}	3.412×10^{-7}
5	1.495×10^{-5}	1.160×10^{-7}
6	1.482×10^{-5}	1.189×10^{-8}

For the smallest value $n = 75$ presented in Table 2, it is found numerically that the contribution to (2.2) corresponding to $k = 2$ is about 11 orders of magnitude smaller than the dominant term with $k = 1$. For the larger n values, this contribution is even smaller and the terms with $k \geq 2$ can be safely neglected. However, for smaller n this is no longer the case and a meaningful approximation has to take into account the contribution from other $k \geq 2$ values.

In Table 3, we illustrate this situation by taking $n = 25$. The second column shows the absolute relative error in the computation of γ_n with $k = 1$ for different truncation index s ; that is, with the approximation $\gamma_n \simeq -\Im J_1$. For $4 \leq s \leq 6$, this error is seen to remain essentially constant at $O(10^{-5})$. The contribution with $k = 2$ is about 5 orders of magnitude smaller than the $k = 1$ contribution, so that this additional contribution needs to be included for larger index s . The absolute relative error including the contribution with $k = 2$ is shown in the third column; that is, with the approximation $\gamma_n \simeq -\Im(J_1 + J_2)$. The expansion with $k = 3$ is about 8 orders of magnitude smaller than the $k = 1$ contribution, so this would only begin to make a significant contribution for $s \geq 6$. This problem becomes even more acute for smaller n values, say $n = 10$,

Table 4: Values for γ_n obtained from (1.1) and (2.13) compared with the exact value.

n	Eq. (1.1)	Eq. (2.13)	Exact γ_n
10	$+2.105395 \times 10^{-4}$	$+2.04713213 \times 10^{-4}$	$+2.05332814 \dots \times 10^{-4}$
50	$+1.275493 \times 10^2$	$+1.26823798 \times 10^2$	$+1.26823602 \dots \times 10^2$
80	$+2.514857 \times 10^{10}$	$+2.51633995 \times 10^{10}$	$+2.51634410 \dots \times 10^{10}$
100	-4.259408×10^{17}	$-4.25340036 \times 10^{17}$	$-4.25340157 \dots \times 10^{17}$
137	$+3.898740 \times 10^{27}$	$-7.99377883 \times 10^{27}$	$-7.99522199 \dots \times 10^{27}$
200	-7.060244×10^{55}	$-6.97465335 \times 10^{55}$	$-6.97464971 \dots \times 10^{55}$
500	$-1.165662 \times 10^{204}$	$-1.16550527 \times 10^{204}$	$-1.16550527 \dots \times 10^{204}$

where higher k values need to be retained. However, the chief interest in the asymptotic expansion in (2.12) is for large n , where this problem is of no real concern.

In Table 4 we show some examples of the asymptotic approximation given in (2.13). We compare these with the values produced by the leading approximation (1.1) and the exact value of γ_n obtained from *Mathematica* using the command `StieltjesGamma[n]`. It will be observed that for $n = 500$ the approximation (2.13) yields nine significant figures.

Finally, we remark that the analysis in Section 2 is immediately applicable to the more general Stieltjes constants $\gamma_n(\alpha)$ appearing in the Laurent expansion for the Hurwitz zeta function $\zeta(s, \alpha)$ about the point $s = 1$. These constants are defined by

$$\zeta(s, \alpha) = \frac{1}{s-1} + \sum_{n=0}^{\infty} \frac{(-)^n}{n!} \gamma_n(\alpha) (s-1)^n,$$

where $\gamma_0(\alpha) = -\Gamma'(\alpha)/\Gamma(\alpha)$ and $\gamma_n(1) = \gamma_n$. It is shown in [7, Eq. (2.9)] that

$$C_n(\alpha) := \gamma_n(\alpha) - \frac{1}{\alpha} e^{n \log \log \alpha} = -\Im \sum_{k=1}^{\infty} e^{-2\pi i k \alpha} J_k.$$

Then it follows that the expansions in Theorems 1 and 2 are modified only in the argument of the trigonometric functions appearing therein, which become $na + b - 2\pi\alpha$. Thus, for example, from (2.13) we have

$$C_n(\alpha) \sim \frac{Be^{nA}}{\sqrt{n}} \left\{ \cos(na+b-2\pi\alpha) \left(1 + \frac{c_1}{n} + \frac{c_2}{n^2} \right) - \sin(na+b-2\pi\alpha) \left(\frac{d_1}{n} + \frac{d_2}{n^2} \right) \right\}$$

as $n \rightarrow \infty$, where the quantities A , B , a , b and the coefficients c_s, d_s ($s = 1, 2$) are as specified in Theorem 2. The leading approximation agrees with that obtained in [7, Eq. (2.4)].

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